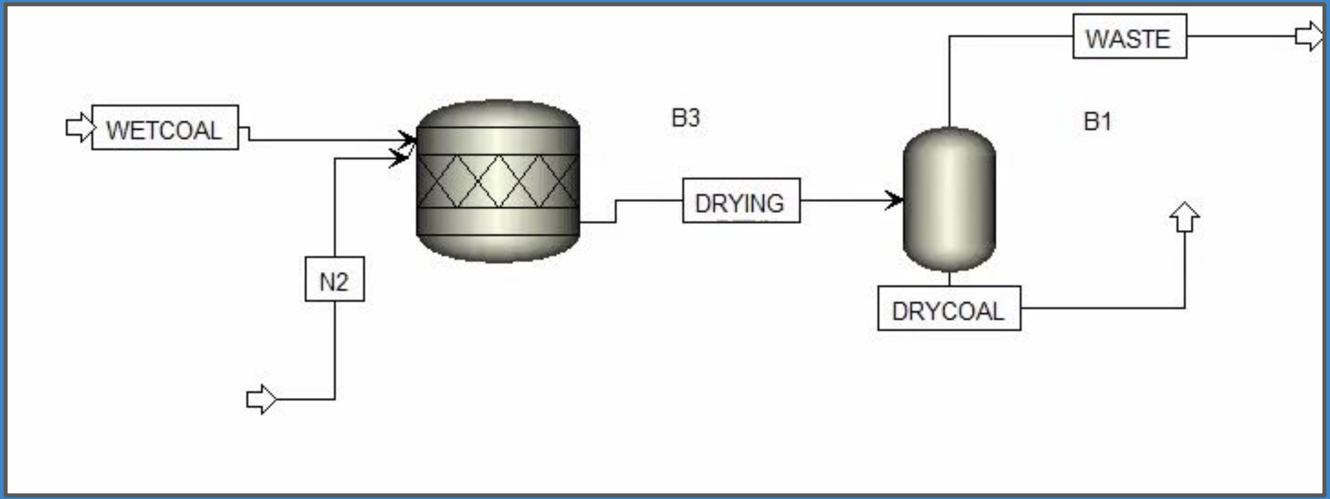
ASPEN Material Balance & Reaction of Custom Compounds

Shon, Zach, Liz, Brian, Amir, Brendon



Material Balance: The Basics

- Material balances are a prerequisite to many essential calculations when considering process design
- The laws of conservation of mass state that mass cannot be created or destroyed, but can only be transferred
- The familiar general form for a material balance is as follows...

$$\textit{Input} - \textit{Output} + \textit{Accumulation} + \textit{Generation} - \textit{Consumption} = 0$$

- Common simplifications include steady-state (accumulation = 0) and no chemical reaction (generation = consumption = 0)

Material Balance: Processes

- **Batch**
  - There is no material exchange during the process itself
- **Continuous**
  - All streams are moving in and out of the system boundaries continuously
- **Semi-Batch**
  - The process has some features of both batch and continuous processes
- **Steady-State vs. Unsteady-State**
  - In a steady-state process, process variables do not depend on time
  - In an unsteady-state process, some or all process variables change depending on when they are measured

Conventional vs. Non-Conventional Inputs

Conventional

- Pure chemical species
- Represented as molecular components
- Examples:
    - Water
    - Methane
    - Ethanol

Non-Conventional

- Solids that are not pure chemical species
- Not represented as molecular components
- Examples:
    - Coal
    - Biomass (wood, EFB, etc.)

Example Problem

$$C_xH_yO_z \cdot nH_2O + Heat + N_2 + O_2 \rightarrow C_xH_yO_z + nH_2O\ (gas)$$

Evaporation of moisture in wet coal using a hot gas stream, often containing nitrogen and oxygen

- Feed involves wet coal with 25% water content
- Goal: Dry coal with 0% water content
- Will have 2 separate water percentages
  - Initial water percentage of wet coal
  - Final water percentage of dry coal

Selecting Components for Aspen Simulation

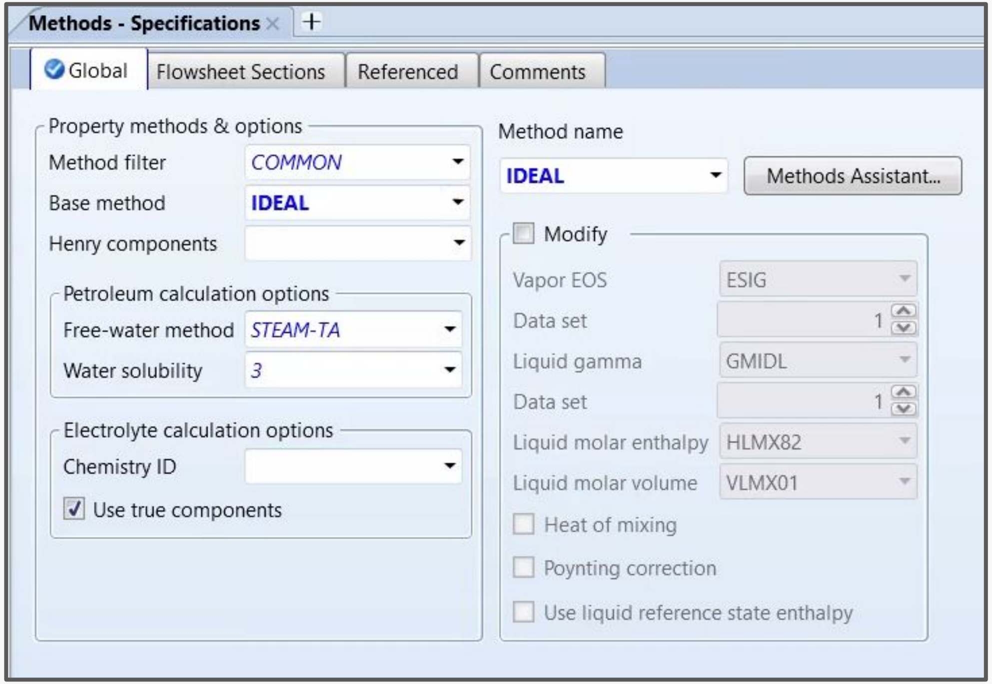
- First step in Aspen - produce material balance
- Can change components throughout process
- Able to define your own compound

Select components

Component ID	Type	Component name	Alias	CAS number
WATER	*Conventional*	WATER	H2O	7732-18-5
NITROGEN	*Conventional*	NITROGEN	N2	7727-37-9
OXYGEN	*Conventional*	OXYGEN	O2	7782-44-7
COAL	Nonconventional			

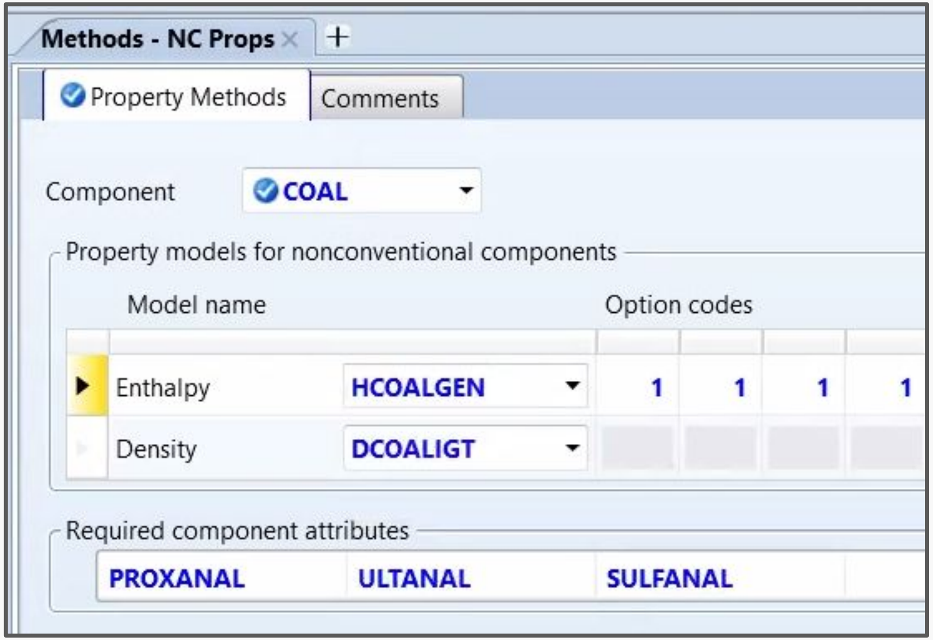
Property Methods

- Ideal, UNIFAC, Wilson
- Used to calculate thermodynamic and transport properties
- Have the ability to manually adjust as well



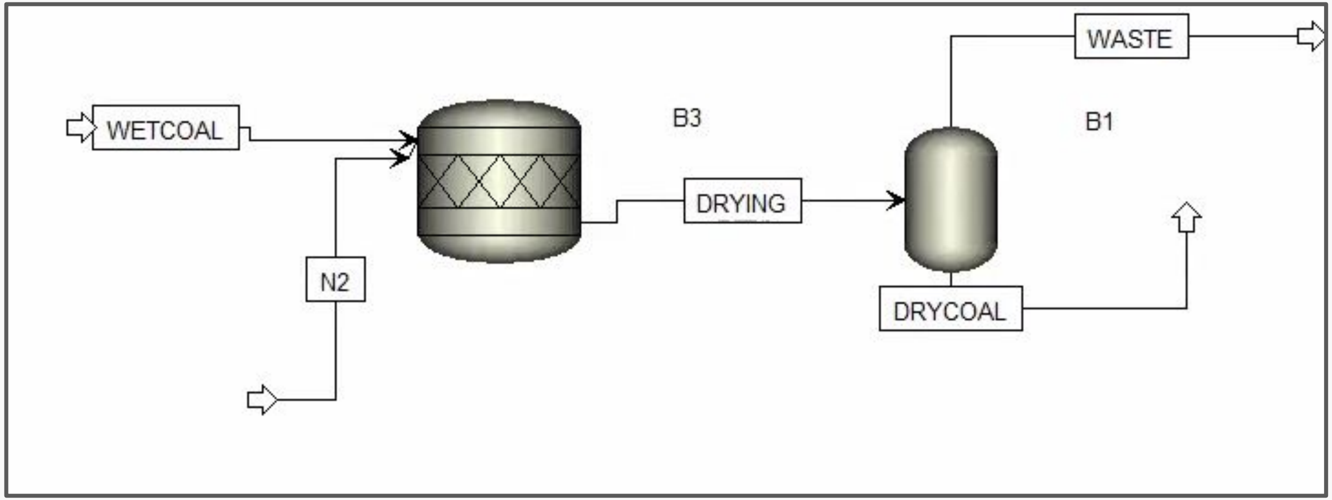
Finalize Methods and Properties

- Helps characterize the unconventional solid and calculate the thermodynamic values
- Last step before running simulation
- Proxanal, Ultanal, Sulfanal: proximate, ultimate and sulfur analysis results



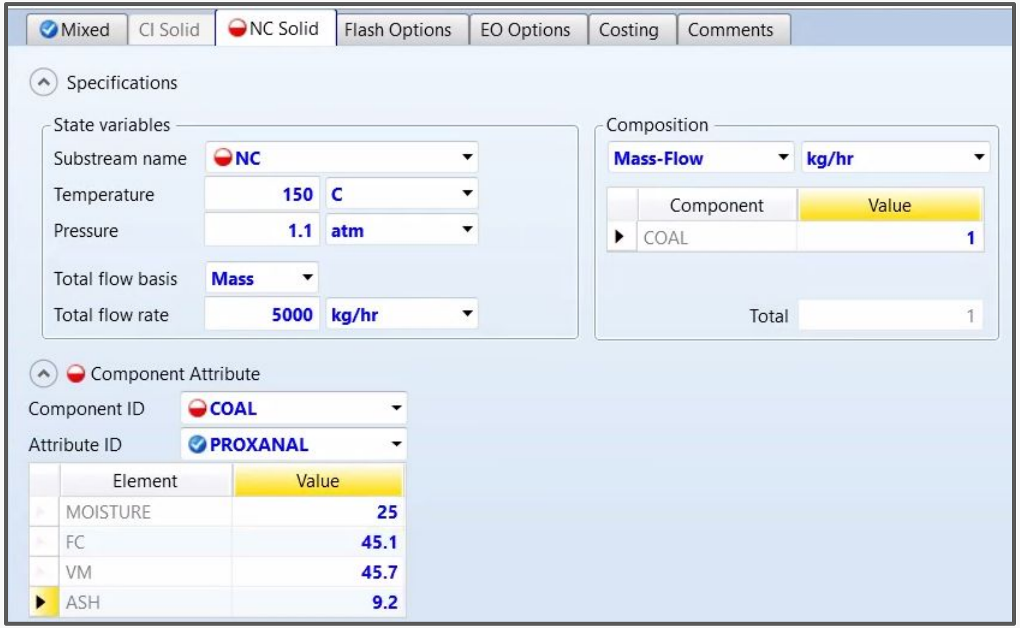
Creating the Reactor and Simulation

- Various blocks to choose from (PFR, heater, mixer, separator)
- Able to add various streams that are material, heat or water
- Add recycle stream to improve purity or recovery



Defining Feed Stream

- Various values to use
  - Will impact recovery and purity
- Have to manually input the value for each element and attribute (proxanal, ultanal, sulfanal)

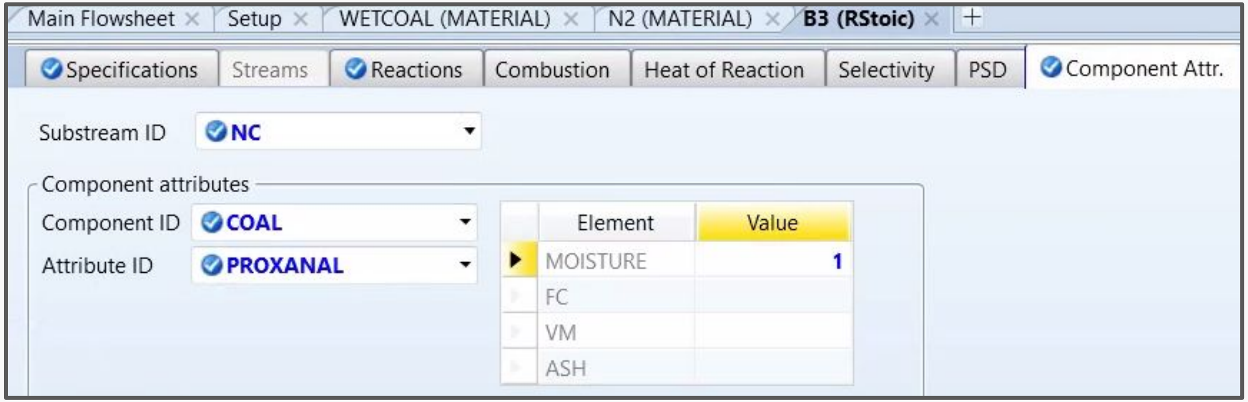


Defining First Reactor Configuration

- Temperature and pressure of reactor is flexible
- Manually enter the equation and stoich
- Purpose is to remove moisture from coal using nitrogen

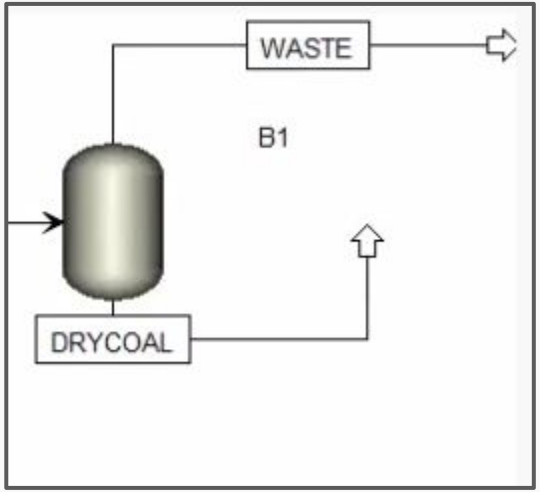
Reactions

Rxn No.	Specification type	Molar extent	Units	Fractional conversion	Fractional Conversion of Component	Stoichiometry
1	*Frac. conversion*		kmol/hr	**0.2**	**COAL**	COAL --> 0.0555084 WATER(MIXED)

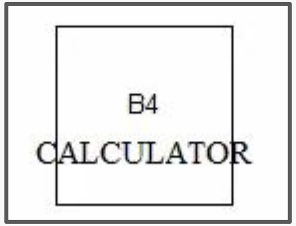


Defining Second Reactor Configuration

- Purpose of second block is to separate waste materials from dry coal
- Want a low pressure to be effective and eco-friendly

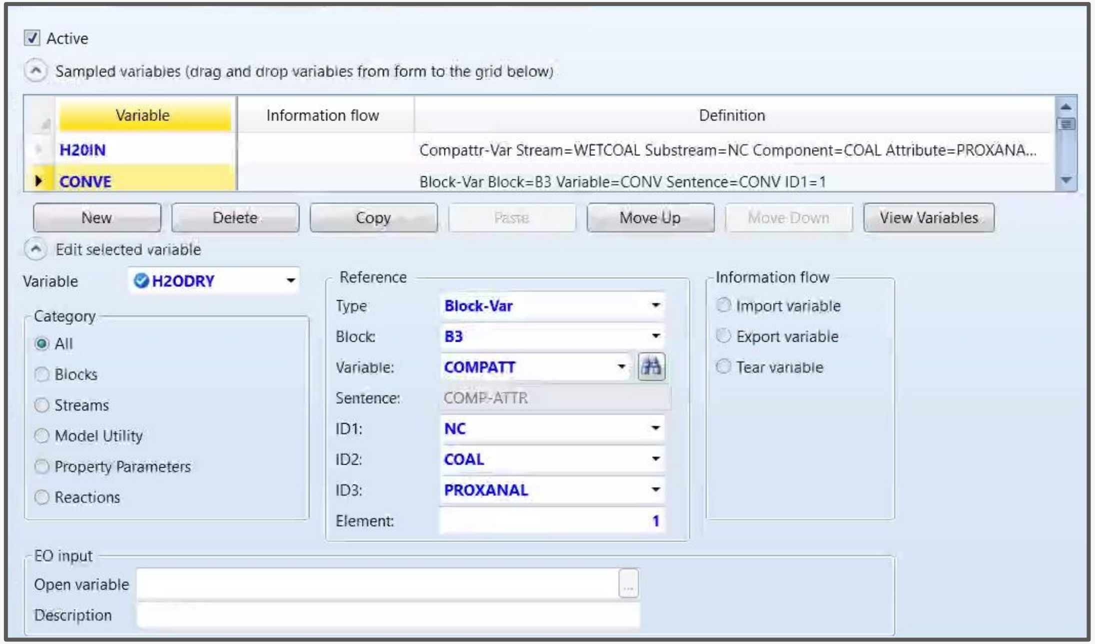


Calculator Block



- Allows you to import equations to calculate the conversion
- Have to manually put in the variables

$$Conver = \frac{H2Oin - H2ODry}{100 - H2ODry}$$



Review of Steps

1. **Select/Input components** (conventional and nonconventional)
2. **Input properties and methods and verify** (Ideal, UNIFAC, or Wilson)
3. **Define feed stream, non-conventional component stream**
4. **Define 1st and 2nd reactor configurations** (setup reaction scheme)
5. **Insert a calculator block** (Allows you to find coefficients)
6. **Run simulation**

Applications

- **Reactor Design** (volume, feed rates, composition of product)
- **Separation Processes** (distillations, extractions, absorptions)
- **Recycle Streams** (minimizing waste, emissions regulations)
- **Custom Formula Compounds $CH_xO_yN_z$** (biomass, coal, cells)
- **Calculating Stoichiometric Coefficients** (aC+bH+cO+dN)

THANK YOU

References

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